Beamlines 8.2.1, 8.2.2, 8.3.1

Multiple-Wavelength Anomalous Diffraction (MAD) and Monochromatic Protein Crystallography

Suite of three protein crystallography beamlines with single superconducting bend magnet as the source

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Suite of Three Protein Crystallography Beamlines with Single Superconducting Bend Magnet as the source.

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INTRODUCTION

At synchrotrons around the world Protein Crystallography beamlines are being built at a rapid pace as it has been realized that this technique can rapidly elucidate protein structures, which can provide one of the foundation blocks for the understanding of life. Many Protein Crystallography beamlines are required as there are many tens of thousands of protein structures to solve. Here at the Advanced Light Source (ALS), a consortium from the Universities of Berkeley and San Francisco have constructed beamline 8.3.1, quickly followed by the Howard Hughes Medical Institute funding the construction of two more identical beamlines (8.2.1 and 8.2.2). All three beamlines are adjacent and use as a source one of the three newly installed 5 Tesla single pole Superconducting-bending magnets. Beamline 8.3.1 is in operation and the other 2 beamlines are finalizing the commissioning process. This document will briefly describe these beamlines and their initial performance.

BEAMLINE DESIGN

Initial work was carried out in 1998 by the University of Berkeley (UCB) group on the test beamline 7.3.3 to determine the feasibility of carrying out Protein Crystallography on regular ALS bending magnets. Complete multiple anomalous dispersive data sets were collected to 1.9Å resolution in ~ 10hours on the non- optimized test beamline [1]. By optimizing the beamline and switching from a regular warm magnet dipole source to a 5 Tesla Superconducting dipole source [2], it would be expected that scan times would drop to ~ 1hour. Speed is increasingly becoming very important for the Protein Crystallography process both due to the large number of protein structures to be solved and the requirement to scan for good samples amongst the many poor ones during the iteration of crystallization procedures.

The simplistic basis for the beamline design was to put as many 6-16 KeV photons through a 100μm diameter pinhole as possible consistent with reasonable cost and robust performance. The optimized beamline design schematic is shown in figure 1. 1.5mrad (h) x 0.5mrad (v) of radiation is accepted by the nickel-plated water-cooled invar mirror (M1), 6.5m from the source. It is shaped into a parabolic cylinder by means of a bending mechanism. Parallel light in the vertical plane is directed into a water-cooled double crystal monochromator (Kohzu

Co.) 18m from the source. The exiting monochromatic light is focused by a toroidal mirror (M2) (21.53m) onto the sample in the hutch with a horizontal demagnification of 2. The end stations are of the mini-hutch type allowing for changing samples by reaching through a sliding door. Ray tracing indicated that using a dipole source size of 230μm (h) x 23μm (v) fwhm resulted in a focused spot size of 150μm (h) x 67μm (v) fwhm with a divergence of 3mrad (h) x 0.33mrad (v).

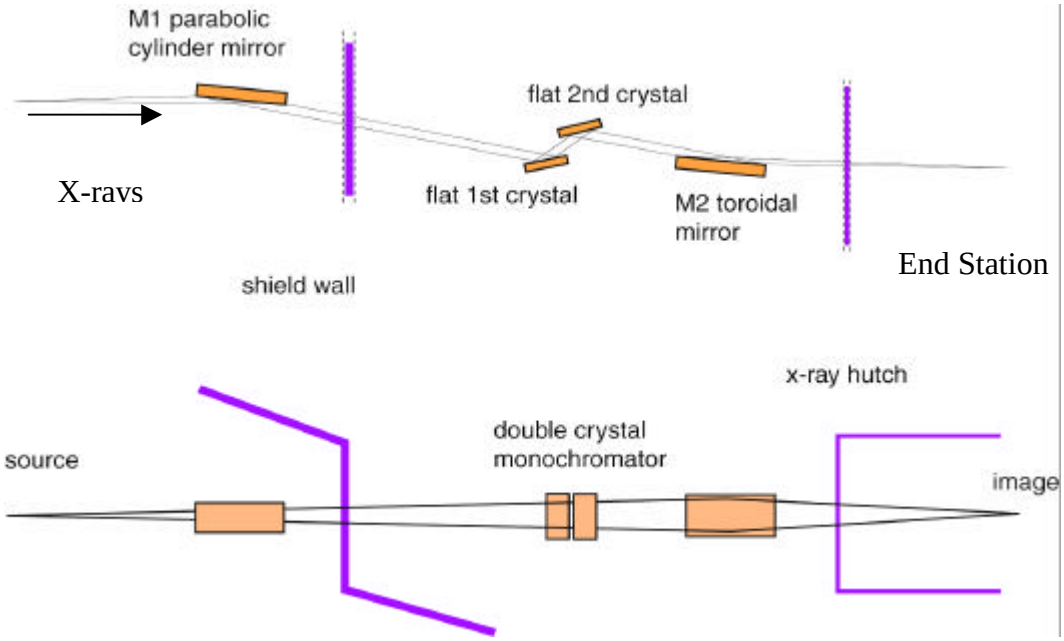

Figure 1. Schematic layout of the new Protein Crystallography Beamlines with a Superbend dipole magnet source. Mirror grazing angles are 4.5mrads.

BEAMLINE PERFORMANCE

The focus spot size at the sample has been measured on the 3 beamlines as ranging from 150μm (h) x 120-160μm (v). This is slightly higher in the vertical than expected and is most likely due to figure and roughness problems that arose during the manufacture of the M1 mirrors. New ones are currently being fabricated. The flux through the 100um pinhole is calculated as 2 x 10^{11} hυ/sec at 12.4KeV (ALS =400mA), but the actual flux measured is less being in the range of 4-8 x 10^{10} hυ/sec at) for the 3 beamlines. This too is expected to improve when the new M1 mirrors are installed. The x-ray convergence angles onto the sample were 1.5mrad (h) x 0.33mrad (v). This is still a very respectable flux and very comparable to the 5.0.2 Protein Crystallography beamline, which uses a 38-pole 2.1 Tesla wiggler magnet insertion device. This is a high power, low brightness source and yields a sample flux of 7x10^{10} hυ/sec at 12.4KeV for the same conditions as used on the Superbend beamlines. This confirms the original concept that the high brightness low power Superbend dipole source can compete with high power low brightness insertion devices for selected applications.
Beamline 8.3.1 has been operational for 2-3 months and has solved 17 structures. Beamlines 8.2.1 and 8.2.2 are undergoing the final commissioning.

REFERENCES

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